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ORIGINAL ARTICLE

Emulating the OPAL equation of state

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Abstract The equation of state for the structure of the Sun and stars has to be precise to allow comparisons with observations, i.e., helioseismic inversions of thermodynamic quantities. Among the two of the most popular formalisms are (1) the OPAL equation of state developed at Livermore and (2) the Mihalas-Hummer-Däppen (MHD) equation of state. While OPAL has a solid theoretical foundation, and matches the observational data better, the MHD formalism is more intuitive, easy to realize, and has the possibility of adjustable parameters. Furthermore, it an open-source product in contrast to the proprietary OPAL. Recently a version of MHD has been obtained by including the so-called "Plank-Larkin partition function" and by adding scattering-state terms. The resulting formalism matches OPAL rather well. Here, we report on the next logical step, the implementation of this MHD upgrade into the simple and popular CEFF equation of state. Such an implementation will make it a flexible and convenient tool, allowing an approximative on-line implementation of OPAL in solar and stellar models.

Keywords Helioseismology · Equation of state · Planck-Larkin partition function

1 Introduction and motivation

The equation of state (EOS) is one of the three key ingredients that constitute any stellar model. Usually, the EOS is highly entangled with the other two material properties, opacity and nuclear reaction rate. Fortunately the development of helioseismology has allowed an isolated study of the EOS, especially in the solar convection zone (Christensen-Dalsgaard 2002). The frequencies of the standing waves observed at the surface of the Sun are closely related to the eigenvalues derived from the solar models. These model oscillation frequencies can be calculated. In numerical inversions, their discrepancy with the corresponding observed frequencies is the input for a calculation of the difference of various physical quantities with respect to the model values. These quantities are localized, that is, obtained as a function of depth. In equation-of-state inversions (Basu and Christensen-Dalsgaard 1997), the quantities are typically a pair such as density and adiabatic sound speed, or density and the adiabatic gradient γ_1. These inversions rely on a linearized relation of the discrepancies of the frequency and physical quantities between observed and modeled data. Given the nature of the method, the equation of state of the model has to be precise and accurate. It has to be precise for the reliability of the numerical inversion, accurate for providing a reference model that is close to the real Sun, so that the linearization assumption is valid.

In order to meet this purpose, there are several recent developments in the EOS. In last 20 years, two EOS have become quite popular for their high precision. They are the so called "MHD" and "OPAL" equations of state, which are both based on a opacity computation efforts, respectively. They are the international Opacity Project (OP) and the OPAL project pursued at Livermore. OP uses the Mihalas-Hummer-Däppen (MHD) equation of state (Hummer and Mihalas 1988; Mihalas et al. 1988; Däppen et al. 1988; Trampedach et al. 2006), which deals with a plasma mixture of all relevant atoms and ions. The ionization equilibrium is found by minimization of the model free energy of the system [the so-called "free-energy minimization method

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(FEMM)]. Since this is analogous to the mass-action law in chemistry, the method of the MHD EOS is said to be realized in the so-called "chemical picture". In contrast, the OPAL project uses an activity-expansion equation of state (ACTEX), referred to as the OPAL EOS (Rogers 1986; Rogers et al. 1996; Rogers and Nayfonov 2002). Its characteristic ingredient is that it is built on the notion of fundamental particles only, that is, electrons and nuclei. For that reason, this realization is said to be in the so-called "physical-picture". Its main advantage is that it provides a systematic method to include nonideal effects, in contrast to the intuitive expressions of the free energy of MHD.

Although both MHD and OPAL EOS are popular because of their high accuracy, they are rather complicated to calculate and so far only available in pre-computed tabular from. Of course that does not preclude the computation of solar and stellar models, but the necessary table interpolations bring in errors and the choice of chemical composition is inflexible since it has to be set at the time of the production of the tables. Therefore, it would be beneficial for application in solar modeling and helioseismology, to have a more convenient numerical tool, which can compute the EOS as a subroutine inside a solar model calculation. For lower accuracy requirements, such tools do exist. The most popular among them is the so called CEFF (Christensen-Dalsgaard and Däppen 1992) equation of state.

CEFF is a derivate of the original EFF EOS, developed by Eggleton, Faulkner and Flannery in 1973 (Eggleton et al. 1973). EFF contains a good treatment of the electrons, based on an analytical function to approximate the Fermi-Dirac integral of partially degenerate electron gas. Even relativistic effects are included. However, pressure ionization is dealt with not with a physical mechanism but a device that guarantees the two correct asymptotic limits (low and high density). The pressure ionization device was introduced from the consideration that the Saha equation alone leads to a spurious recombination at very high density for any temperature. In EFF, this spurious recombination is removed by giving the ground state of bound species (such as hydrogen atoms) a statistical weight of the form of $\exp(-a_0^3/r^3 - a_0^2/r_D^2)$, where r_D is the Debye radius and r is the mean inter-electron distance. Note that this is a purely *ad-hoc* device, but it leads to the desired asymptotic behavior. In addition, is only a ground-state contribution included in the internal partition function. Because of its simplicity, the EFF EOS can be directly incorporated into the programs of solar evolution or helioseismology. In 1992, Christensen-Dalsgaard and Däppen upgraded EFF to CEFF by including the Coulomb interactions. Even today, because of its flexibility and formal precision, it is still a widely used tool serving in reference model for helioseismology.

Therefore, in order to incorporate more detailed physics, a highly-developed EOS such as OPAL or MHD is needed. But in order to make them useful and practical, the best would be to mimic their behavior inside a simple phenomenological but versatile computational tool such as CEFF.

When it comes to comparisons with observations, it turns out that models with the OPAL equation of state yield a closer match to reality than those with the MHD equation of state (Däppen, *these proceedings*). However, since MHD is realized in the chemical picture, with intuitive free-energy expressions, there is actually still room for adjustments to bring it closer to OPAL. Such adjustments have been successfully made. A modification of MHD by Aihua Liang and Dan Mao (Liang 2004; Däppen and Mao 2009), dubbed OPAL emulator, shows a very good agreement with OPAL. This is a good first step, but its usefulness is still limited by the table nature of MHD. To complete the task, these modifications have to be carried over from MHD into CEFF. Only then the OPAL emulator becomes a practically useful tool.

2 Research goal and progress

As mentioned above, our ultimate goal is a modification of CEFF to achieve an OPAL emulation. While our procedure will follow the successful earlier modification of MHD, we now show that the procedure done in MHD cannot be simply carried over to CEFF. Here we briefly describe how the modifications that were made in MHD and the strategy for doing the analog for CEFF.

The modifications in MHD consist of two parts. The key role is played on the one hand by the so-called Planck-Larkin partition function (PLPF),

$$\mathrm{PLPF} = \sum_{nl}(2l+1)\exp\left(-\frac{E_{nl}}{k_B T}\right) - 1 + \frac{E_{nl}}{k_B T}$$

and on the other hand by the scattering terms (which physically arise when free particles are not treated by plane waves but true continuum, in other words, scattering states).

$$F_{ep} = -2N_e N_p \frac{k_B T}{V}\left(\frac{-\pi}{3}\right)(\beta e^2)^3\left(\ln\frac{\Lambda_{ep}}{\lambda_D} + D_q\right),$$

$$F_{ee} = -N_e^2\frac{k_B T}{V}\Bigg\{2\pi\int_0^\infty [e^{\beta q(r)} - 1]r^2 dr - \frac{\hbar^2}{m_e}\frac{\pi}{6}\beta^3 \times \int_0^\infty e^{\beta q(r)}\left[-q(r)\left(\frac{1}{r} + \frac{1}{\lambda_D}\right)\right]^2 r^2 dr + 2\pi\lambda_D^2(\beta e^2) - \frac{\pi}{2}\lambda_D(\beta e^2)^2\Bigg\},$$

$$F_{pp} = -N_p^2 \frac{k_B T}{V} 2\pi \left\{ \int_0^\infty [e^{\beta q(r)} - 1] r^2 dr + 2\pi \lambda_D^2 (\beta e^2) - \frac{\pi}{2} \lambda_D (\beta e^2)^2 \right\},$$

$$q(r) = \frac{e^2}{r} e^{-r/\lambda_D}$$

with Λ_{ep} being the thermal de Broglie wavelength divided by $\sqrt{4\pi}$, $\Lambda_{ep} = \hbar/\sqrt{2\mu_{epk_B T}}$, λ_D the Debye-Hückel radius $\sqrt{\epsilon_0 k_B T B / e^2 (N_e + Z_p^2 N_p)}$, and the constant $D_q = 0.8872$.

The two parts of the prior modifications of MHD are:

- First, the PLPF was implemented by replacing the standard internal partition functions of the MHD formalism. The PLPF is convergent without the occupation-probability weights used in MHD. We should bear in mind that such a procedure is purely *ad hoc*, and not the result of a consistent theory within the chemical-picture approach. The procedure is justified as a means to achieve the OPAL emulation.
- Second, higher-order terms corresponding to the continuum-state 2-body Coulomb-interactions are included. These terms, often denoted as 'scattering-states terms', have no analog in the traditional chemical-picture formalism which is based on plane-wave continuum states. Its implementation is consistent with our choice of the PLPF.

Though we can see the success of the emulation of OPAL EOS based on a modification of the MHD equation of state (see Fig. 1), there are still technical problems remaining to be solved before we can emulate OPAL using CEFF. There are several reasons for this. First, CEFF itself is by itself different from MHD due to a simpler physics, lacking for instance MHD's detailed treatment of bound states. In MHD, hundreds of excited states are included for each ionized species. In CEFF all ions are assumed to be in their ground states.

Since the CEFF equation of state has been already widely applied in stellar modeling and successfully tested by the community, its coding and efficiency can be considered reliable. The strategy of changing CEFF will consist of adding scattering states and the PLPF.

3 Numerical results and conclusions

Figure 2 shows the difference in pressure for 4 different equation-of-state models with respect to OPAL, in the sense model—OPAL (the horizontal zero line thus being OPAL). The 4 models are:

- MHD: the MHD EOS.
- CEFF: the CEFF EOS.
- MHD(scattering-only): the MHD EOS with the extra scattering terms.
- CEFF(scattering-only): the CEFF EOS with the extra scattering terms.

The figure reveals the difference between the CEFF and MHD equation of state, which will have to be dealt with in a successful emulation of OPAL using CEFF. The figure

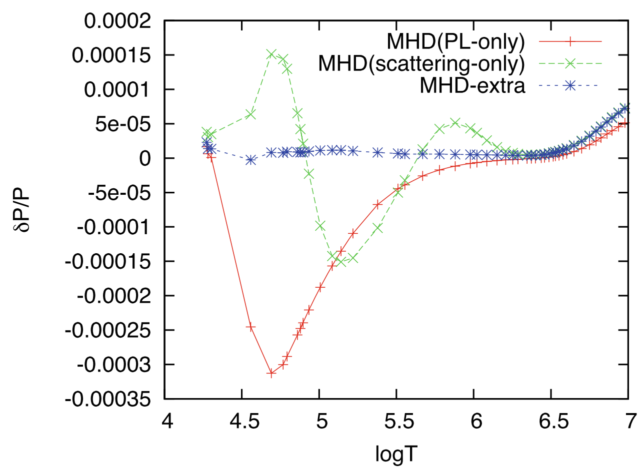

Fig. 1 Difference in pressure for selected equation-of-state models with respect to OPAL, in the sense model—OPAL (the *horizontal zero line* thus being OPAL). MHD (PL-only) and MHD (scattering-only) are modifications of the original MHD, one with the Planck-Larkin partition function, the other with scattering terms, respectively. The resulting combination of both modifications (here named MHD-extra) lies close to OPAL

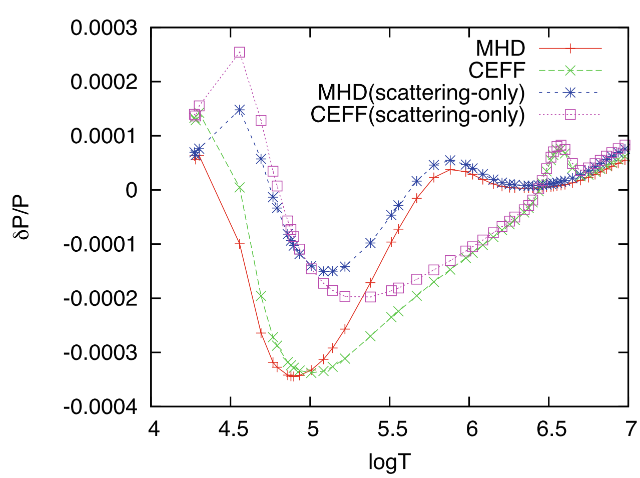

Fig. 2 Same as Fig. 1, but also comparing CEFF models. First, MHD and CEFF are compared with OPAL, showing that their difference forces us to use a different procedure when OPAL is emulated from within CEFF rather than MHD. Second, a further complication arises from the fact that the inclusion of scattering terms has quite a different effect in CEFF and MHD, as displayed by MHD (scattering-only) and CEFF (scattering-only). A successful emulation of OPAL based on CEFF will have to take into account this discrepancy

also shows the result of adding scattering terms to CEFF, which is different from the result of adding the scattering terms to MHD (Fig. 1). Therefore, in order to achieve our ultimate goal of emulating the OPAL equation of state using the CEFF formalism, we cannot simply carry over the procedure that achieves the emulation with MHD. On the one hand, we will have to make an extra effort to build in the difference between MHD and CEFF. On the other hand, we will also have to compensate for the different effect that adding scattering states has in MHD and CEFF, respectively. Finally, the PLPF will have to be introduced into CEFF. Since quite generally, the net result of a PLPF is not too different from a simple ground-state-only formalism (Rogers 1986), intuitively, in CEFF we expect a smaller change due to PLPF than in MHD. This work is in progress.

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